REPORT

SECOND TEAM WORKSHOP

MATERIALS RESEARCH IN AN ABERRATION-FREE ENVIRONMENT

July 18 - 19, 2002
Lawrence Berkeley National Laboratory

It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are. The only trouble is that the electron microscope is one hundred times too poor … I put this out as a challenge: Is there no way to make the electron microscope more powerful?

– Richard P. Feynman, 1959, "There's Plenty of Room at the Bottom"

PREFACE

A revolutionary breakthrough in electron optics has created the opportunity to observe directly the atomic-scale order, electronic structure, and dynamics of individual nanoscale structures – all with atomic spatial resolution. This breakthrough consists of the development, for the first time, of aberration-correcting electron optics, which dramatically improve the achievable numerical aperture in electron optical systems and remove the barrier that has limited the performance of the electron microscope since its invention. The resulting improvement in the *spatial resolution*, *contrast*, *sensitivity*, and *flexibility of design* of electron optical instruments will create unprecedented scientific opportunities through:

- Direct observation of the three-dimensional atomic-scale structure, shape, and defect distribution of individual nanostructures via atomic resolution tomography;
- Spectroscopic identification, with single-atom sensitivity, of individual dopants or impurities, and their location within crystalline nanostructures on specific substitutional or interstitial lattice sites, or their segregation to surfaces or defects;
- Direct imaging, for the first time, of the atomic-scale structures of glasses;
- Atomic-resolution characterization of the electronic structure of individual point defects and electronically distinct sites in nanostructures;
- Measurement of non-spherical charge density and valence electron distribution;
- Synthesis of novel nanoscale structures by direct electron-beam lithographic removal of individual atomic columns;
- In-situ observation of the synthesis of individual nanostructures with atomic or near-atomic spatial resolution;
- In-situ observation of processing methods, such as thin film growth, oxidation, and deformation at atomic or near-atomic spatial resolution; and
- In-situ scientific investigation of dynamical materials responses to variations in external thermodynamic variables, such as temperature, pressure, stress, chemical activity, and applied electric and magnetic fields with unprecedented temporal resolution at atomic or near-atomic spatial resolution.

In his famous 1959 lecture, “There’s Plenty of Room at the Bottom,” Nobel Laureate Richard P. Feynman anticipated that the ability to directly image the atomic-scale structure of molecular-scale objects, no matter how complex, would provide a physical basis for predicting their properties. The connection between atomic-scale structure and properties will be fully developed during the coming decades at the nanometer scale, where the frontier of theory, modeling and simulation rises to meet that of the most powerful experimental characterization methods. New physical principles govern materials behavior at the nanoscale, where quantum mechanics dominate and electronic structure transforms from bulk-like to molecular-like behavior. However, the basic physics and chemistry of materials at the nanoscale remain largely unexplored. Such basic solid-state concepts as densities of states, thermodynamics, and transport mechanisms need to be defined. Theory, modeling and simulation will play an important role in uncovering this science; however, the properties of nanoscale objects are strongly dependent upon the subtleties of their atomic-scale structure, including their size, shape, and defect distributions. *Atomic-scale imaging plays a* ***unique*** *role in defining the quantum mechanical boundary conditions needed to perform the electronic structure calculations required to understand how nanostructures work.*

SPONSORING ORGANIZATIONS

Second Transmission Electron Aberration-corrected Microscopy (TEAM) Workshop: Materials Research in an Aberration-free Environment

July 18-19, 2002
Lawrence Berkeley National Laboratory

Electron Microscopy Center (EMC)
Argonne National Laboratory

National Center for Electron Microscopy (NCEM)
Lawrence Berkeley National Laboratory

Center for the Microanalysis of Materials (CMM)
Frederick-Seitz Materials Research Laboratory

Shared Research Equipment Program (SHaRE)
Oak Ridge National Laboratory

WORKSHOP PROGRAM

DAY 1 - JULY 18

8:15 - 8:20 Welcoming Remarks from LBNL - P.M. Oddone
8:20 - 8:25 Introductory Remarks from DOE - A.H. Carim
8:25 - 8:30 Welcome and Introduction - U. Dahmen
8:30 - 9:00 Recent Breakthroughs with Electron Microscopy - J.C.H. Spence

Session I: Scientific Challenges
Chair: U. Dahmen, NCEM, LBNL

9:00 - 9:30 Scientific Challenges in Nanomaterials - M.S. Dresselhaus
9:30 - 10:00 Computational Materials Science - T. Diaz de la Rubia

*10:00 - 10:30 ** coffee break ***

Session II: Scientific Challenges, continued
Chair: I.M. Anderson, SHaRE, ORNL

10:30 - 11:00 Solid State Lighting – M.G. Craford
11:00 - 11:30 Scientific Issues in Magnetic Recording - H.C. Siegmann
11:30 - 12:00 Issues of Scale in Semiconductor Materials - D.J. Eaglesham

*12:00 – 1:30 ** lunch ***

Session III: The Promise of Aberration Correction
Chair: D. Miller, EMC, ANL

1:30 - 2:15 Opportunities for Aberration Corrected Electron Microscopy - J. Silcox
2:15 - 2:30 Aberration Correctors for Electron Optics: The State of the Art - M. Haider
2:30 - 2:45 Aberration Correctors for STEM: The State of the Art - O.L. Krivanek
2:45 - 3:00 Electron Optical Designs for TEAM - B. Kabius

*3:00 - 3:30 ** coffee break ***

Session IV: Application Areas of Electron Microscopy
Chair: I. Petrov, CMM, FSMRL

3:30 - 4:00 Electron Microscopy of Interfaces - N.D. Browning
4:00 - 4:30 Electron Microscopy in Catalysis - P.L. Gai
4:30 - 5:00 Electron Microscopy of Superconducting and Magnetic Nanoparticles - J. Zweck
5:00 - 5:30 Electron Microscopy of Deformation and Defects - P. Pirouz

DAY 2 - JULY 19

Session V: Application Areas of Electron Microscopy, continued
Chair: U. Dahmen, NCEM, LBNL

8:30 - 9:00 Electron Beam Tomography - K.H. Downing
9:00 - 9:30 In-situ Microscopy: Reaction Mechanisms and Dynamics - F.M. Ross

Session VI: Breakout Sessions
Chair: I.M. Anderson, SHaRE, ORNL

9:30 - 9:35 Remarks in advance of breakout sessions - A.H. Carim
9:35 - 9:45 Instructions to participants concerning breakout sessions - R.M. Tromp
9:45 - 10:45 Break-out sessions to discuss proposed projects:
feedback from the scientific community - C.B. Carter, J.A. Eades, R. Sinclair

*10:45 - 11:00 ** coffee break ***

11:00 - 12:00 Break-out sessions to discuss proposed projects:
feedback from the scientific community - J.C.H. Spence, J. Silcox, R.M. Tromp
12:00 -12:30 Summary of break-out sessions
High Resolution - C.B. Carter
Analytical - J.A. Eades
In Situ - R. Sinclair

*** Close of Public Workshop ***

2:00 - 4:00 TEAM Advisory Committee meeting

EXECUTIVE SUMMARY

A revolution is occurring in electron optics. This consists of the development, for the first time, of aberration-correction devices for electron-beam instruments. This development is certain to produce a quantum leap in the performance, and allow considerable flexibility in the design, of charged particle optical instruments that fuel progress in many fields of science, from photoemission microscopes used at the synchrotron X-ray light sources to electron-beam lithography tools, from focused ion beam instruments to scanning electron microscopes. In no field is the promise of aberration-corrected charged particle optics greater than in the area of atomic and near-atomic imaging, spectroscopy, and in-situ measurements of dynamical processes in the transmission electron microscope (TEM). It is this field that was the concern of this workshop. However, the performance requirements for atomic-scale imaging are exceptionally stringent, and the added complexity of aberration-corrected TEMs demands that any investment must involve careful planning for the design, maintenance, and development of this technology. *The U.S. Department of Energy (DOE) is unique among public and private institutions in its mission and capacity to make the necessary investment to develop, to maintain, and to ensure the broad impact of this advancement.* This document describes the scientific opportunities and payoff to be expected from such an investment.

Materials science challenges at the nanometer scale herald the approach of a critical juncture in the development of many key technologies in the U.S. and world economies, and for maintaining national security. For example, the shrinkage to near-molecular dimensions of gate dielectrics and other key features in integrated circuits will soon bring to an impasse the predictable evolutionary improvements in information technologies that result from the scaling down of a relatively fixed circuit architecture. New *revolutionary* concepts will be required to sustain the Moore's Law rate of improvement in computing power, and almost without exception materials development issues are central to sustained progress in this $200 billion per year industry. Materials development issues are also pivotal in the migration of mature technologies to improved high-tech paradigms. For example, the vast majority of the one-hundred-fold cost reduction necessary to effect a transition from vacuum-tube-based lighting to solid-state lighting via high power light-emitting diodes (LEDs) can be achieved through materials improvements alone. Achieving the 150 lumens/watt efficiency goal of the proposed ten-year National Lighting Initiative would cut in half the power consumption for lighting, which is estimated to result in a ten percent reduction in overall power consumption.

In the face of these enormous materials challenges, the potential for novel solutions has never been greater, given the exciting developments in nanoscale science and technology. New physical principles govern materials behavior at the nanoscale, where quantum mechanics dominate and electronic structure transforms from bulk-like to molecular-like behavior. However, the basic physics and chemistry of materials at the nanoscale remain largely unexplored. Such basic solid-state concepts as densities of states, thermodynamics, and transport phenomena, and their dependence upon atomic-scale structure, need to be defined. Theory will play an important role in uncovering this science, as computational methods are becoming sufficiently powerful to simulate materials behavior at this scale. However, experiment in general, and effective characterization in specific, are needed both to uncover the science inaccessible to computational modeling, and to validate theoretical predictions.

Transmission electron microscopy is uniquely suited to the atomic-scale spatial, temporal, and electronic characterization of *individual* nanostructures. *This can be accomplished by no other competing technique.* While scanning tunneling, atomic force, and related scanned probe microscopes have played an important role in nanoscale science, these methods can only probe the surfaces, cannot reveal the three-dimensionality, and have insufficient temporal resolution to study the dynamics, of nanoscale objects. The powerful DOE-funded synchrotron X-ray and neutron sources, which will clearly have an important role in nanoscale science, are best suited to the statistical characterization of ensembles of nanostructures; practical limitations arise when the specimen volume is insufficient to generate adequate signal. For example, X-ray crystallography methods require the synthesis of macroscopic quantities of nanoscale structures; direct imaging of individual nanostructures circumvents this requirement. Along these lines, a recent achievement of electron microscopy has been the discovery of the three-dimensional structure of the ribosome, responsible for protein synthesis, the most fundamental process for life on earth. Realistic atomic-scale structures are also essential for quantitative interpretation of diffraction data acquired from larger ensembles of such structures, for example small angle scattering data acquired at the nation's synchrotron and neutron sources.

More fundamentally, atomic-scale imaging plays a unique role in defining the quantum mechanical boundary conditions needed to perform the electronic structure calculations necessary to understand how nanostructures work. A recent illustration is the in-situ synthesis of the ultimate nanowire, comprised of discrete atomic chains of gold atoms that give rise to quantum conductance. This example illustrates a recent coming of age in electron microscopy: *Quantitative TEM has now matured to the point that studies go beyond the acquisition of images and spectra to uncover the underlying physics and chemistry of matter, thereby elucidating functionality and behavior.* Notable successes include: mapping the cloud of bonding electrons in copper oxide (cuprite), thereby revealing the dz^2 orbital shape of a charge hole and metal-metal bonds (joint electron and X-ray diffraction study); spatially resolving the variation in electronic structure in boron solute-segregated and solute-free regions of a single grain boundary in Ni_3Al, thereby explaining the beneficial effect of boron additions on alloy ductility; and the in-situ observation of changes of shape (faceted, rounded, or flat) of copper nanoparticles, used as fuel cell catalysts, in response to different gas environments.

The enormous potential of aberration-correcting electron optics for establishing new scientific opportunities is unmistakable. Aberration-correcting devices retrofitted to existing TEMs in a few laboratories around the world have already demonstrated unprecedented imaging performance, and there is every reason to believe that this represents the leading edge of a new era in electron optical imaging. The conventional (CTEM) and scanning (STEM) approaches to TEM each provide unique scientific opportunities. For example, in the field of catalysis, CTEM can provide time-resolved imaging of structural variations of individual catalyst particles at atomic resolution during in-situ perturbation of external thermodynamic variables such as temperature or partial pressures, while STEM can probe the electronic structure of individual chemically active sites. Atomic resolution tomography with either instrument configuration can reveal the three-dimensional atomic structure, shape, and defect distribution in nanoscale catalyst particles. Similar advances can be expected for the characterization of the structure and chemistry of interfaces and other defects, glasses, deformation, thin-film growth, corrosion, and functional materials such as ferroelectrics and superconductors.

Aberration-correction also provides improved contrast and sensitivity because of the resulting higher numerical aperture of the electron lens. This improved sensitivity provides a significant advantage for applications limited by signal-to-noise, for example the characterization of beam-sensitive soft materials and biomaterials. Alternatively, the improved contrast and sensitivity can be traded for improved performance elsewhere in the electron optical column. For example, the order of magnitude improvement in beam current resulting from a factor of three increase in the incident beam divergence can be used to compensate for the corresponding order of magnitude decrease that results from improved monochromation of the incident electron probe; aberration-correction can thereby be used to effect improved spectral resolution in STEM or an improved information limit in CTEM without loss of signal-to-noise.

Perhaps the greatest potential impact of aberration-correcting electron optics is the improved flexibility in instrument design for in-situ studies of dynamical processes of materials. For such in-situ studies, ultimate spatial resolution might be somewhat sacrificed to achieve greater space in the vicinity of the specimen, *allowing the microscope to be effectively transformed into a compact self-contained materials science laboratory*. With an instrument design featuring greater space in the vicinity of the specimen, it is anticipated that individual scientists could seek to address specific scientific questions by developing custom experimental modules that could be inserted into the electron optical column. MEMS device technologies and microlithographic techniques could be used to take best advantage of the available space in the specimen area. The potential impact of aberration-corrected electron optics in this area of in-situ dynamical studies of materials generated particular enthusiasm in the breakout sessions by workshop participants.

The substantial cost of developing and maintaining these unique aberration-corrected electron microscopes suggests limiting investments to a few national or regional centers. Until now it has been normal and appropriate for electron microscopes, with a cost of the order of $1 million, to be acquired by individual investigators. However, an investment several times this amount would be required to acquire the column alone for an aberration-corrected electron microscope *designed to operate at the limits of its performance*. An instrument designed to achieve the full potential performance of the aberration-correcting optics is distinct from the hybrid instruments operating or on order today, in which an aberration-correction device has been interfaced to an earlier generation microscope, even though these have or will display strong performance by today's standard. Substantial further investments would be required for the instrument development necessary to enable the broad-based scientific investigation outlined here. An additional investment of the order of the cost of the instrument will be required to provide a sufficiently "quiet" site, free of electromagnetic fields and vibrations, to house such instruments. Given the increased complexity of these advanced aberration-corrected microscopes, significant operating funds will also be required to develop these instruments to a point where they routinely achieve their ultimate performance, and thereafter to maintain the instruments at their performance limits with acceptable levels of reliability and availability. It is anticipated that these national or regional centers will develop the instrumentation as regards peripheral equipment, such as specimen stages, experimental modules and advanced detectors, in order to tailor the instrumentation to high-impact scientific investigations.

The BES-sponsored electron beam microcharacterization centers (EBMCs) are well positioned to provide leadership in the development of this remarkable new technology for broad-based scientific investigation. Effective user access will be critical for maximizing the scientific impact of such a national resource following the initial development phase of the instrumentation. The four EBMCs sponsored by the DOE Office of Basic Energy Sciences (BES), located at Argonne National Laboratory, the Frederick-Seitz Materials Research Laboratory, Lawrence Berkeley National Laboratory and Oak Ridge National Laboratory, all have well-established user programs with missions that are aligned with BES science goals. In addition, the EBMCs have achieved a significant level of coordination over the past several years in pursuit of the development of the electron beam microcharacterization user centers in general, and the Transmission Electron Aberration-corrected Microscope (TEAM) project in particular. This record of cooperation provides a good foundation for the development of the TEAM project, which will require an unprecedented level of collaboration and common purpose within the electron microscopy community as a whole in order to succeed. Significant contributions are to be expected from additional partner institutions, such as Brookhaven National Laboratory, that are similarly aligned with BES science goals and located within the context of major materials research and development efforts. Stewardship of this major new initiative will add an important new role to the function of the EBMCs, and care must be taken to ensure that the substantial support currently provided to both general and specialized users of these centers is maintained during the development of this new national resource.

Now is the time for a significant investment in next-generation aberration-corrected electron microscopes. The recent breakthrough in aberration-correcting electron optics, the maturing of electron microscopy in support of broad-based scientific investigation, the advent of the National Nanotechnology Initiative, and the importance of materials development to sustain progress in national defense and important sectors of the U.S. economy: all point to the timeliness of this investment. Accordingly, the TEAM Advisory Committee, comprised of national leaders in electron microscopy, has urged the Electron Beam Microcharacterization Centers to immediately develop a proposal outlining a major new initiative in aberration-corrected electron microscopy. The Advisory Committee recommends that the Centers accelerate the processes of engaging the general scientific community and building consensus within the electron microscopy community in order to formulate a strategic plan that will maximize the impact of aberration-corrected electron microscopy on the scientific progress of the nation. *Just as DOE's investment in synchrotron sources at a few well supported centers significantly improved the rate of scientific progress through advancing the state of the art of X-ray scattering methods, so too will an investment in aberration-corrected electron microscopy establish a new era in electron optical characterization, creating new scientific opportunities that are inaccessible by any other means*.

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